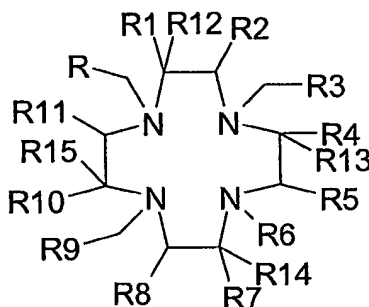


We claim:

1. A compound comprising a polyazamacrocyclic compound and at least one phosphonic group substituted on at least one of the aza groups of said polyazamacrocyclic compound.

2. The compound of claim 1 wherein said polyazamacrocyclic compound comprises the general formula (II):



(II)

where  $R^1 = R^2 = R^7 = R^8 = R^{10} = R^{11} = H$ ;

$R^{12}, R^{13}, R^{14}, \text{ and } R^{15} = CH_3 \text{ or } H$ ;

$R^4 = R^5$ ; and  $R^{10} = R^{11}$  can be H or groups taken together forming a cyclic C<sub>3</sub>-C<sub>4</sub> alkene group;

at least one of R, R<sup>3</sup>, R<sup>6</sup> or R<sup>9</sup> = X, where X = CH<sub>2</sub>P(O)(OH)<sub>2</sub>, CH<sub>2</sub>P

(O)(OC<sub>4</sub>H<sub>9</sub>-t)<sub>2</sub>, CH<sub>3</sub>CH P(O)(OH)<sub>2</sub>, CH P(O)(OH)<sub>2</sub>-

(CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>H, CH P(O)(OH)<sub>2</sub>, (CH<sub>2</sub>)<sub>n</sub>NH<sub>2</sub>, CH P(O)(OH)<sub>2</sub>-

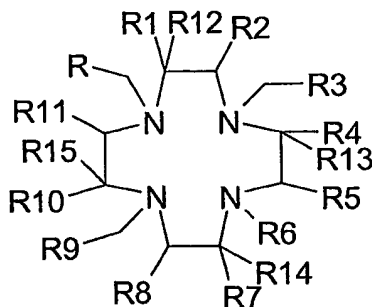
Aryl-CO<sub>2</sub>H, CH P(O)(OH)<sub>2</sub>-Aryl-NH<sub>2</sub> or CHP(O)(OH)<sub>2</sub>-

Aryl-NHCS, where n= 1-12; and

when R, R<sup>3</sup>, R<sup>6</sup> or R<sup>9</sup> are not X, then that R, R<sup>3</sup>, R<sup>6</sup> or R<sup>9</sup> is CO<sub>2</sub> C

(CH)<sub>3</sub>, or CO<sub>2</sub>H.

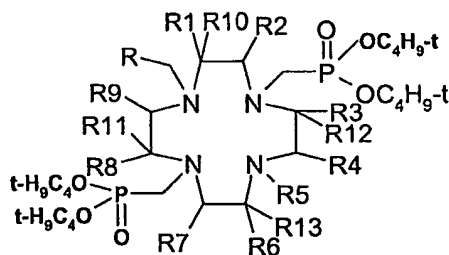
3. The compound of claim 1 wherein said polyazamacrocyclic compound comprises the general formula (III):



(III)

- 5 where  $R = R^3 = R^9 = \text{CO}_2\text{C}(\text{CH}_3)_3$ , or  $\text{CO}_2\text{H}$ ;  
 $R^1 = R^2 = R^4 = R^5 = R^7 = R^8 = R^{10} = R^{11} = \text{H}$ ;  
 $R^{12}, R^{13}, R^{14}$ , and  $R^{15} = \text{CH}_3$  or  $\text{H}$ ;  
 $R^{10} = R^{11}$  can be  $\text{H}$  or groups taken together forming a cyclic  $\text{C}_3\text{-C}_4$   
 alkene group; and  
 10  $R^6 = \text{CH}_2\text{P}(\text{O})(\text{OH})_2$ ,  $\text{CH}_2\text{P}(\text{O})(\text{OC}_4\text{H}_9\text{-t})_2$ ,  $\text{CH}_3\text{CHP}(\text{O})(\text{OH})_2$ ,  $\text{CH}$   
 $\text{P}(\text{O})(\text{OH})_2\text{-(CH}_2)_n\text{CO}_2\text{H}$ ,  $\text{CHP}(\text{O})(\text{OH})_2$ ,  $(\text{CH}_2)_n\text{NH}_2$ ,  $\text{CHP}$   
 $(\text{O})(\text{OH})_2\text{-Aryl-CO}_2\text{H}$  or  $\text{CHP}(\text{O})(\text{OH})_2\text{-Aryl-NH}_2$ , where  $n$   
 $= 1\text{-}12$ .

4. The compound of claim 1 wherein said polyazamacrocyclic compound  
 15 comprises the general formula (IV):



(IV)

where  $R^1 = R^2 = R^3 = R^4 = R^6 = R^7 = R^8 = R^9 = \text{H}$ ;

$R^3 = R^4$  and  $R^8 = R^9$  can be H or groups taken together forming a cyclic C<sub>3</sub>-C<sub>4</sub> alkene group;

$R^{10}, R^{11}, R^{12}$  and  $R^{13} = CH_3$  or H;

$R = CO_2C(CH_3)_3$ ; and

5  $R^5 = CH_2P(O)(OH)_2, CH_2P(O)(OC_4H_9-t)_2, CH_3CHP(O)(OH)_2,$   
 $CHP(O)(OH)_2-(CH_2)_nCO_2H, CHP(O)(OH)_2, (CH_2)_nNH_2,$   
 $CHP(O)(OH)_2-Aryl-CO_2H, CHP(O)(OH)_2-Aryl-NH_2$  or  $CH$   
 $P(O)(OH)_2-Aryl-NHCS$ , where  $n = 1-12$ .

5. A compound of the formula:

10 10-Phosphonomethyl-1,4,7,10-tetraazacyclododecane-1,4,7-triacetic  
 acid (MPDO3A);  
 10-(1-phosphonoethyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triacetic  
 acid;  
 10-[[Bis(1,1-dimethylethoxy)phosphinyl]methyl]-1,4,7,10-  
 15 tetraazacyclododecane-1,4,7-triacetic acid 1,7-bis(1,1-  
 dimethylethyl)ester;  
 10-[[Bis(1,1-dimethylethoxy)phosphinyl]methyl]- $\alpha'$ -(carboxymethyl)-  
 1,4,7,10-tetraazacyclododecane-1,4,7-triacetic acid  $\alpha, \alpha', \alpha''$ -  
 tris(1,1-dimethylethyl)ester;  
 20 10-[[1-[Bis(1,1-dimethylethoxy)phosphinyl]-3-carboxy]propyl]-  
 1,4,7,10-tetraazacyclododecane-1,4,7-triacetic  $\alpha, \alpha', \alpha''$ -tris(1,1-  
 dimethylethyl)ester; or  
 4,10-Bis[[bis(1,1-dimethylethoxy)phosphinyl]methyl]-1,4,7,10-  
 tetraazacyclododecane-1,7-diacetic (1,1-dimethylethyl)ester.

25 6. A compound comprising a homo dimer, hetero dimer, homo multimer or  
 hetero multimer of the compound of any of claims 1-5.

7. A complex comprising the compound of any of claims 1-5 complexed with a paramagnetic or radionuclide metal.

8. A method for preparing a complex comprising the step of conjugating the compound of any of claims 1-5 with a paramagnetic or radionuclide metal.

5 9. A method of imaging comprising the steps of:  
administering to a patient a diagnostic imaging agent comprising the compound of any of claims 1-5 complexed with a paramagnetic or radionuclide metal, and imaging said patient.

10 10. A method for preparing a diagnostic imaging agent comprising the step of adding to an injectable medium a substance comprising the compound of any of claims 1-5.

11. A kit for preparing a diagnostic imaging agent comprising the compound of any of claims 1-5.

12. A kit for preparing a radiotherapeutic agent comprising the compound of any of claims 1-5.

15 13. A method of treating a patient comprising the step of administering to a patient a radiotherapeutic agent comprising the compound of any of claims 1-5 complexed with a therapeutic radionuclide.

14. A method of preparing a radiotherapeutic agent comprising the step of adding to an injectable therapeutic medium a substance comprising at least one compound of any of  
20 claims 1-5.

15. The compound of any of claims 1-5 further comprising a linking group.

16. The complex of claim 7 further comprising a linking group.

17. The compound of any of claims 1-5 further comprising a targeting moiety.

18. The complex of claim 7 further comprising a targeting moiety.

19. The compound of any of claims 1-5 further comprising a linking group and a targeting moiety.

20. The complex of claim 7 further comprising a linking group and a targeting moiety.

5 21. A salt form of the compound of any of claims 1-5.

22. A salt form of the complex of claim 7.

23. A method for preparing a polyazamacrocyclic compound bound to a linker, targeting moiety, diagnostic moiety or therapeutic moiety comprising the step of:

conjugating a polyazamacrocyclic compound to a linker, targeting moiety,

10 diagnostic moiety or therapeutic moiety with a coupling agent, wherein:

said coupling agent is selected from the group consisting of DCC, HOBT and

HATU,

said polyazamacrocyclic compound comprises one carboxyl group and/or at

least one amino group, and

15 said linker, targeting moiety, diagnostic moiety or therapeutic moiety

comprises at least one amino or acid functional group.